Controllability of the Schroedinger equation via adiabatic methods and conical intersections of the eigenvalues

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***Abstract*— We present a constructive method to control the bilinear Schrödinger equation by means of two or three controlled external fields. The method is based on adiabatic techniques and works if the spectrum of the Hamiltonian admits eigenvalue intersections, with respect to variations of the controls, and if the latter are conical. We provide sharp estimates of the relation between the error and the controllability time.**

I. Introduction

In this paper we are interested in the problem of controlling the bilinear Schrödinger equation

$$i\frac{d\psi}{dt} = \left(H_0 + \sum_{k=1}^{m} u_k(t)H_k\right)\psi(t). \tag{1}$$

Here ψ belongs to the Hilbert sphere $\mathbf{S}$ of a (finite or infinite dimensional) complex separable Hilbert space $\mathcal{H}$ and $H_0,\dots,H_m$ are self-adjoint operators on $\mathcal{H}$. The controls $u_1,\dots,u_m$ are scalar-valued and represent the action of external fields. H_0 describes the "internal" dynamics of the system, while $H_1,\dots,H_m$ the interrelation between the system and the controls.

When describing quantum phenomena, typical models have often the previous form with $H_0 = -\Delta + V_0(x)$, $H_i = V_i(x)$, where x belongs to a domain $D \subset \mathbb{R}^n$ and $V_0,\dots,V_m$ are real functions (multiplication operators). However, equation (1) can be used to describe more general controlled dynamics. For instance, a quantum particle on a Riemannian manifold subject to external fields or a two-level ion trapped in a harmonic potential (the so-called Eberly–Law model [1], [5]). In the latter case, as in many other relevant physical situations, H_0 cannot be written as the sum of a Laplacian plus a potential.

The controllability problem aims at establishing whether, for every pair of states ψ_0 and ψ_1, there exist controls $u_k(\cdot)$ and a time T such that the solution of (1) with initial condition $\psi(0)=\psi_0$ satisfies $\psi(T)=\psi_1$. The answer to this question is in general negative when $\mathcal{H}$ is infinite-dimensional (see [2], [20]). Hence one has to look for weaker controllability properties as, for instance, approximate controllability (see for instance [7], [9], [13], [15]) or controllability between subfamilies of states and in particular the eigenstates of H_0 (which are the most relevant physical states) and other regular states (see [3], [4]).

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In most of the results in the literature only the case $m = 1$ is considered. In this paper we study the cases $m = 2, 3$ and we look both for controllability results and explicit expressions of the external fields realizing the transition. The system under consideration is then

$$i\frac{d}{dt}\psi(t) = H(\mathbf{u}(t))\psi(t),$$

with $H(\mathbf{u}) = H_0 + \sum_{i=1}^{m} u_i H_i,\ m = 2,3$ and $\mathbf{u} = (u_1,\dots,u_m)$. The idea is to use slowly varying controls and climb the energy levels through conical intersections, if they are present.

A classical tool, which is used in our approach, is the adiabatic theorem (see [19]). Roughly speaking, the adiabatic theorem states that the occupation probabilities associated with the energy levels of a time-dependent Hamiltonian $H(\cdot)$ are almost preserved along the evolution given by $i\dot{\psi}(t) = H(t)\psi(t)$, provided that $H(\cdot)$ varies very slowly. This result works whenever the energy levels (i.e. the eigenvalues of $H(\cdot)$) are pairwise isolated for every t. On the other hand, if $H(\cdot)$ is a $\mathcal{C}^2$ slowly varying Hamiltonian, the passage through (conical) intersections among energy levels determine (approximate) exchanges of the corresponding occupation probabilities (see [19, Corollary 2.5] and Figure 1). In this paper we generalize this property in order to construct suitable paths allowing to approximately attain prescribed distributions of probability, thus getting a particular controllability property (that we call approximate spread controllability). The case $m = 2$ has already been studied in [8]. In this paper we will tackle the case $m = 3$. For reasonable space reasons, all the results will be presented without proof. As for the case $m = 3$ they can be obtained by suitably adapting the proofs in [8]. This case will be analyzed in more details in future works.

The structure of the paper is the following. In Section II, we introduce the framework and we state the main result. In Section III we recall the time adiabatic theorem and some results on the regularity of eigenvalues and eigenstates of parameter-dependent Hamiltonians. In Section IV we deepen our analysis of conical intersection; in particular, we state and prove a sufficient condition for an intersection to be conical. Our first controllability result is introduced in Section V, while Section VI is devoted to the construction, under additional assumptions, of some special curves that allow to strengthen our controllability result.

II. Definitions and notations

We consider the Hamiltonian

$$H(\mathbf{u}) = H_0 + \sum_{i=1}^{m} u_i H_i,$$

for $\mathbf{u} = (u_1,\dots,u_m) \in \mathbb{R}^m$. From now on we assume that $H(\cdot)$ satisfies the following assumption:

(H0) H_0 is a self-adjoint operator on a separable Hilbert space $\mathcal{H}$, and H_i are bounded self-adjoint operators on $\mathcal{H}$ for $i = 1,\dots,m$.

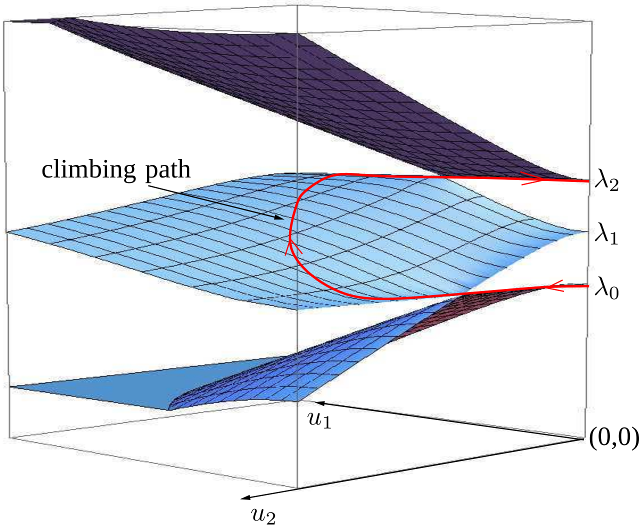

Fig. 1. A slow path "climbing" the spectrum of $H(\cdot)$, plotted in function of $\mathbf{u} = (u_1, u_2)$.

Some of the results of this paper, in particular those in the last section, are obtained in the case where $m = 3$, denoted in the following with $(\mathbf{C})$, or in the following case

(R) Assume that $m = 2$ and that there exists an orthonormal basis $\{\chi_j\}_j$ of the Hilbert space $\mathcal{H}$ such that the matrix elements $\langle \chi_j, H_0 \chi_k \rangle$, $\langle \chi_j, H_1 \chi_k \rangle$ and $\langle \chi_j, H_2 \chi_k \rangle$ are real for any j, k. We denote with $\mathcal{H}^{\mathbb{R}}$ the real Hilbert space generated by the basis $\{\chi_j\}_j$.

Remark 2.1: In the case **(R)**, with each $\mathbf{u}$ and each eigenvalue of $H(\mathbf{u})$ (counted according to their multiplicity), it is possible to associate an eigenstate whose components with respect to the basis $\{\chi_j\}_j$ are all real.

Concerning the case **(R)**, a typical example is when $H_0 = -\Delta + V$, where Δ is the Laplacian on a bounded domain $\Omega \subset \mathbb{R}^d$ with Dirichlet boundary conditions, $V \in L^\infty(\Omega, \mathbb{R})$, $\mathcal{H} = L^2(\Omega, \mathbb{C})$, and H_1, H_2 are two bounded multiplication operators by real valued functions. In this case the spectrum of H_0 is discrete. However the case **(R)** does not cover some basic quantum systems, as for instance the electromagnetic Hamiltonian, in which one controls the magnetic field. Although this system is not linear in the controls, the results presented in this paper for the case **(C)** have to be intended as a first step towards the complete analysis of the electromagnetic case.

The dynamics are described by the time-dependent Schrödinger equation

$$i \frac{d\psi}{dt} = H(\mathbf{u}(t))\psi(t). \tag{2}$$

Such an equation has classical solutions under hypothesis **(H0)**, $\mathbf{u}(\cdot)$ piecewise $\mathcal{C}^1$ and with an initial condition in the domain of H_0 (see [18] and also [2]).

We are interested in controlling (2) inside some portion of the discrete spectrum of $H(\mathbf{u})$. Since we use adiabatic techniques, such portion of spectrum must be well separated from its complement in the spectrum of the Hamiltonian, and this property must hold uniformly for $\mathbf{u}$ belonging to some domain in $\mathbb{R}^m$. All these properties are formalized by the following notion.

Definition 2.2: Let ω be a domain in $\mathbb{R}^m$. A map Σ defined on ω that associates with each $\mathbf{u} \in \omega$ a subset $\Sigma(\mathbf{u})$ of the discrete spectrum of $H(\mathbf{u})$ is said to be a *separated discrete spectrum* on ω if there exist two continuous functions $f_1, f_2 : \omega \to \mathbb{R}$ such that

- $f_1(\mathbf{u}) < f_2(\mathbf{u})$ and $\Sigma(\mathbf{u}) \subset [f_1(\mathbf{u}), f_2(\mathbf{u})] \qquad \forall \mathbf{u} \in \omega$.
- there exists $\Gamma > 0$ such that

$$\inf_{\mathbf{u}\in\omega} \inf_{\lambda \in \mathrm{Spec}(H(\mathbf{u}))\setminus\Sigma(\mathbf{u})} \mathrm{dist}(\lambda, [f_1(\mathbf{u}), f_2(\mathbf{u})])) > \Gamma.$$

Notation From now on we label the eigenvalues belonging to $\Sigma(\mathbf{u})$ in such a way that $\Sigma(\mathbf{u}) = \{\lambda_0(\mathbf{u}), \dots, \lambda_k(\mathbf{u})\}$, where $\lambda_0(\mathbf{u}) \leq \dots \leq \lambda_k(\mathbf{u})$ are counted according to their multiplicity (note that the separation of Σ from the rest of the spectrum guarantees that k is constant). Moreover we denote by $\phi_0(\mathbf{u}), \dots, \phi_k(\mathbf{u})$ an orthonormal family of eigenstates corresponding to $\lambda_0(\mathbf{u}), \dots, \lambda_k(\mathbf{u})$. Notice that in this notation λ_0 does not need to be the ground state of the system.

Definition 2.3: Let Σ be a separated discrete spectrum on ω. We say that (2) is approximately *spread-controllable* on Σ if for every $\mathbf{u}^0, \mathbf{u}^1 \in \omega$ such that $\Sigma(\mathbf{u}^0)$ and $\Sigma(\mathbf{u}^1)$ are non-degenerate, for every $\bar{\phi} \in \{\phi_0(\mathbf{u}^0), \dots, \phi_k(\mathbf{u}^0)\}$, $p \in [0,1]^{k+1}$ such that $\sum_{l=0}^k p_l^2 = 1$, and every $\varepsilon > 0$ there exist $T > 0$, $\vartheta_0, \dots, \vartheta_k \in \mathbb{R}$ and a piecewise $\mathcal{C}^1$ control $\mathbf{u}(\cdot) : [0, T] \to \mathbb{R}^m$ such that

$$\|\psi(T) - \sum_{j=0}^{k} p_j e^{i\vartheta_j} \phi_j(\mathbf{u}^1)\| \leq \varepsilon, \tag{3}$$

where $\psi(\cdot)$ is the solution of (2) with $\psi(0) = \bar{\phi}$.

Our techniques rely on the existence of conical intersections between the eigenvalues. Notice indeed that when two levels intersect the conservation of occupation probabilities of the concerned levels under adiabatic evolution is no more guaranteed. Conical intersections constitute a well-known notion in molecular physics (see for instance [6], [12], [19]).

In this paper we will use the following definition, which meets all the features commonly attributed to conical intersections.

Definition 2.4: Let $H(\cdot)$ satisfy hypothesis **(H0)**. We say that $\bar{\mathbf{u}} \in \mathbb{R}^m$ is a *conical intersection* between the eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$ has multiplicity two and there exists a constant $c > 0$ such that for any unit vector $\mathbf{v} \in \mathbb{R}^m$ and $t > 0$ small enough we have that

$$\lambda_{j+1}(\bar{\mathbf{u}} + t\mathbf{v}) - \lambda_j(\bar{\mathbf{u}} + t\mathbf{v}) > ct\,. \tag{4}$$

It is worth noticing that conical intersections are not pathological phenomena. On the contrary, they often happen to be generic, as explained in [8].

III. Survey of Basic Results

A. The adiabatic theorem

One of the main tools used in this paper is the adiabatic theorem ([6], [10], [14], [16]); here we recall its formulation, adapting it to our framework. For a general overview see the monograph [19]. We remark that we refer here exclusively to the time-adiabatic theorem.

The adiabatic theorem deals with quantum systems governed by Hamiltonians that explicitly depend on time, but whose dependence is slow. While in quantum systems driven by time-independent Hamiltonians the evolution preserves the occupation probabilities of the energy levels, this is in general not true for time-dependent Hamiltonians. The adiabatic theorem states that if the time-dependence is slow, then the occupation probability of the energy levels, which also evolve in time, is approximately conserved by the evolution.

More precisely, consider $h(t) = H_0 + \sum_{i=1}^m u_i H_i$, $t \in I = [t_0, t_f]$, satisfying **(H0)**, and assume that the map $t \mapsto \mathbf{u}(t) = (u_1(t), \dots, u_m(t))$ belongs to $\mathcal{C}^2(I, \mathbb{R}^m)$. Assume moreover that there exists $\omega \subset \mathbb{R}^m$ such that $\mathbf{u}(t) \in \omega$ for all $t \in I$ and Σ is a separated discrete spectrum on ω.

We introduce a small parameter $\varepsilon > 0$ that controls the time scale, and consider the slow Hamiltonian $h(\varepsilon t)$, $t \in [t_0/\varepsilon, t_f/\varepsilon]$. The time evolution (from t_0/ε to t) $\widetilde{U}^\varepsilon(t, t_0/\varepsilon)$ generated by $h(\varepsilon \cdot)$ satisfies the equation $i\frac{d}{dt}\widetilde{U}^\varepsilon(t, t_0/\varepsilon) = h(\varepsilon t)\widetilde{U}^\varepsilon(t, t_0/\varepsilon)$. Let $\tau = \varepsilon t$ belong to $[t_0, t_f]$ and $\tau_0 = t_0$; the time evolution $U^\varepsilon(\tau, \tau_0) := \widetilde{U}^\varepsilon(\tau/\varepsilon, \tau_0/\varepsilon)$ satisfies the equation

$$i\varepsilon \frac{d}{d\tau} U^\varepsilon(\tau, \tau_0) = h(\tau) U^\varepsilon(\tau, \tau_0). \tag{5}$$

Notice that $U^\varepsilon(\tau, \tau_0)$ does not preserve the probability of occupations: in fact, if we denote by $P_*(\tau)$ the spectral projection of $h(\tau)$ on $\Sigma(\mathbf{u}(\tau))$, then $P_*(\tau)U^\varepsilon(\tau, \tau_0)$ is in general different from $U^\varepsilon(\tau, \tau_0)P_*(\tau_0)$.

Let us consider the *adiabatic Hamiltonian* associated with Σ, $h_a(\tau) = h(\tau) - i\varepsilon P_*(\tau)\dot{P}_*(\tau) - i\varepsilon P_*^\perp(\tau)\dot{P}_*^\perp(\tau)$, where $P_*^\perp(\tau) = \mathrm{id} - P_*(\tau)$ and id denotes the identity on $\mathcal{H}$. Here and in the following the time-derivatives shall be intended with respect to the reparametrized time τ. The adiabatic propagator associated with $h_a(\tau)$, denoted by $U_a^\varepsilon(\tau, \tau_0)$, is the solution of

$$i\varepsilon \frac{d}{d\tau} U_a^\varepsilon(\tau, \tau_0) = h_a(\tau) U_a^\varepsilon(\tau, \tau_0), \qquad U_a^\varepsilon(\tau_0, \tau_0) = \mathrm{id}.$$

Notice that $P_*(\tau)U_a^\varepsilon(\tau, \tau_0) = U_a^\varepsilon(\tau, \tau_0)P_*(\tau_0)$, that is, the adiabatic evolution preserves the occupation probability of the band Σ.

Now we can adapt to our setting the strong version of the quantum adiabatic theorem, as stated in [19].

Theorem 3.1: Assume that $H(\mathbf{u}) = H_0 + \sum_{i=1}^m u_i H_i$ satisfies **(H0)**, and that Σ is a separated discrete spectrum on $\omega \subset \mathbb{R}^m$. Let $I = [t_0, t_f]$, $\mathbf{u} : I \to \omega$ be a $\mathcal{C}^2$ curve and set $h(t) = H(\mathbf{u}(t))$. Then $P_* \in \mathcal{C}^2(I, \mathcal{L}(\mathcal{H}))$ and there exists a constant $C > 0$ such that for all $\tau, \tau_0 \in I$

$$\|U^\varepsilon(\tau, \tau_0) - U_a^\varepsilon(\tau, \tau_0)\| \leq C\varepsilon\left(1 + |\tau - \tau_0|\right). \tag{6}$$

Remark 3.2: If there are more than two parts of the spectrum which are separated by a gap, then it is possible to generalize the adiabatic Hamiltonian as ([14]) $h_a(\tau) = h(\tau) - i\varepsilon \sum_\alpha P_\alpha(\tau)\dot{P}_\alpha(\tau)$, where each $P_\alpha(\tau)$ is the spectral projection associated with a separated portion of the spectrum, partitioning it as α varies.

Let us now consider the band made by the eigenvalues $\lambda_j, \lambda_{j+1} \in \Sigma$. There exists an open domain $\omega' \subset \omega$ such that $\{\lambda_j, \lambda_{j+1}\}$ is a separated discrete spectrum on ω'. As above, we consider a control function $\mathbf{u}(\cdot) \in \mathcal{C}^2(I, \omega')$. We can then apply the adiabatic theorem to the separated discrete spectrum $\Sigma' : \mathbf{u} \mapsto \{\lambda_j(\mathbf{u}), \lambda_{j+1}(\mathbf{u})\}$, $\mathbf{u} \in \omega'$: we call $\mathfrak{H}(\tau)$ the space constituted by the direct sum of the eigenspaces relative to $\lambda_j(\mathbf{u}(\tau)), \lambda_{j+1}(\mathbf{u}(\tau))$.

We are interested in the dynamics inside $\mathfrak{H}(\tau)$. Since $\mathfrak{H}(\tau)$ is two-dimensional for any τ, it is possible to map it isomorphically on $\mathbb{C}^2$ and identify an *effective Hamiltonian* whose evolution is a representation of $U_a^\varepsilon(\tau, \tau_0)|_{\mathfrak{H}(\tau_0)}$ on $\mathbb{C}^2$.

Let us assume that there exists an eigenstate basis $\{\phi_\alpha(\tau), \phi_\beta(\tau)\}$ of $\mathfrak{H}(\tau)$ such that $\phi_\alpha(\cdot), \phi_\beta(\cdot)$ belong to $\mathcal{C}^1(I, \mathcal{H})$. We construct the time-dependent unitary operator $\mathcal{U}(\tau) : \mathfrak{H}(\tau) \to \mathbb{C}^2$ by defining for any $\psi \in \mathfrak{H}(\tau)$ $\mathcal{U}(\tau)\psi = e_1\langle\phi_\alpha(\tau), \psi\rangle + e_2\langle\phi_\beta(\tau), \psi\rangle$, where $\{e_1, e_2\}$ is the canonical basis of $\mathbb{C}^2$, and the *effective propagator* $U_{\mathrm{eff}}^\varepsilon(\tau, \tau_0) = \mathcal{U}(\tau)U_a^\varepsilon(\tau, \tau_0)\mathcal{U}^*(\tau_0)$. It is easy to see that $U_{\mathrm{eff}}^\varepsilon(\tau, \tau_0)$ satisfies the equation

$$i\varepsilon \frac{d}{d\tau} U_{\mathrm{eff}}^\varepsilon(\tau, \tau_0) = H_{\mathrm{eff}}^\varepsilon(\tau) U_{\mathrm{eff}}^\varepsilon(\tau, \tau_0),\ U_{\mathrm{eff}}^\varepsilon(\tau_0, \tau_0) = \mathrm{id},$$

where $H_{\mathrm{eff}}^\varepsilon(\tau)$ is the *effective Hamiltonian* whose form is

$$H_{\mathrm{eff}}^\varepsilon(\tau) = \begin{pmatrix} \lambda_\alpha(\tau) & 0 \\ 0 & \lambda_\beta(\tau) \end{pmatrix} - i\varepsilon \begin{pmatrix} \langle\phi_\alpha(\tau), \dot{\phi}_\alpha(\tau)\rangle & \langle\phi_\beta(\tau), \dot{\phi}_\alpha(\tau)\rangle \\ \langle\phi_\alpha(\tau), \dot{\phi}_\beta(\tau)\rangle & \langle\phi_\beta(\tau), \dot{\phi}_\beta(\tau)\rangle \end{pmatrix}. \tag{7}$$

Theorem 3.1 implies the following.

Theorem 3.3: Assume that $\{\lambda_j, \lambda_{j+1}\}$ is a separated discrete spectrum on ω' and let $\mathbf{u} : [t_0, t_f] \to \omega'$ be a $\mathcal{C}^2$ curve such that there exists a $\mathcal{C}^1$-varying basis of $\mathfrak{H}(\cdot)$ made of eigenstates of $h(\cdot)$. Then there exists a constant C such that

$$\begin{aligned} \| \left(U^\varepsilon(\tau, \tau_0) - \mathcal{U}^*(\tau)U_{\mathrm{eff}}^\varepsilon(\tau, \tau_0)\mathcal{U}(\tau_0)\right)|_{\mathfrak{H}(\tau)}(\tau_0)\| \\ \leq C\varepsilon(1 + |\tau - \tau_0|) \end{aligned}$$

for every $\tau, \tau_0 \in [t_0, t_f]$.

B. Regularity of eigenstates

Classical results (see [17]) say that the map $\mathbf{u} \mapsto P_\mathbf{u}$, where $P_\mathbf{u}$ is the spectral projection relative to a separated discrete spectrum, is analytic on ω. In particular, eigenstates relative to simple eigenvalues can be chosen analytic with respect to $\mathbf{u}$. Similar results hold also for intersecting eigenvalues, provided that the Hamiltonian depends on one parameter and is analytic. In particular, if Σ is a separated discrete spectrum on ω and $\mathbf{u} : I \to \omega$ is analytic, then there exist two families of analytic functions $\Lambda_j : I \to \mathbb{R}$ and $\Phi_j : I \to \mathcal{H}$, $j = 0, \ldots, k$, such that for every t in I the $(k+1)$-tuple $(\Lambda_0(t), \ldots, \Lambda_k(t))$ is a reordering of $(\lambda_0(u(t)), \ldots, \lambda_k(u(t)))$, and $(\Phi_0(t), \ldots, \Phi_k(t))$ is an orthonormal basis of corresponding eigenstates. (see [11], [17, Theorem XII.13]). Moreover, we can easily find conditions on the derivatives of the functions Λ_l, Φ_l: indeed, consider a $\mathcal{C}^1$ curve $\mathbf{u} : I \to \mathbb{R}^m$ such that there exist two families of $\mathcal{C}^1$ functions $\Lambda_l : I \to \mathbb{R}$ and $\Phi_l : I \to \mathcal{H}$, $l = 0, \ldots, k$, which for any $t \in I$, correspond to the eigenvalues and the (orthonormal) eigenstates of $H(\mathbf{u}(t))$.

By direct computations we obtain that for all $t \in I$ the following equations hold:

$$\dot{\Lambda}_l(t) = \langle\Phi_l(t), \Big(\sum_{i=1}^m \dot{u}_i(t)H_i\Big)\Phi_l(t)\rangle \tag{8}$$

$$\begin{aligned} &(\Lambda_m(t) - \Lambda_l(t))\,\langle\Phi_l(t), \dot{\Phi}_m(t)\rangle = \\ &= \langle\Phi_l(t), \Big(\sum_{i=1}^m \dot{u}_i(t)H_i\Big)\Phi_m(t)\rangle. \end{aligned} \tag{9}$$

An immediate consequence of (8) is that the eigenvalues λ_l are Lipschitz with respect to t.

Let $\bar{\mathbf{u}}$ be a conical intersection between $\lambda_j(\mathbf{u})$ and $\lambda_{j+1}(\mathbf{u})$. Consider the straight line $r_\mathbf{v}(t) = \bar{\mathbf{u}} + t\mathbf{v}$, $t \geq 0$, $\mathbf{v} = (v_1, \ldots, v_m)$ unit vector. Then (9) implies that

$$\lim_{t \to 0^+} \langle\phi_j(r_\mathbf{v}(t)), \Big(\sum_{i=1}^m v_i H_i\Big)\phi_{j+1}(r_\mathbf{v}(t))\rangle = 0. \tag{10}$$

IV. Conical intersections

In this section, we investigate the features of conical intersections and provide also a criterion for checking if an intersection between two eigenvalues is conical. First of all we notice that Definition 2.4 can be reformulated by saying that an intersection $\bar{\mathbf{u}}$ between the eigenvalues λ_j and λ_{j+1} is conical if and only if there exists $c > 0$ such that, for every straight line $r(t)$ with $r(0) = \bar{\mathbf{u}}$, it holds

$$\frac{d}{dt}\Big|_{t=0^+}\Big[\lambda_{j+1}(r(t)) - \lambda_j(r(t))\Big] \geq c.$$

Moreover, the following result guarantees that (4) holds true in a neighborhood of a conical intersection. It follows easily from the Lipschitz continuity of the eigenvalues.

Lemma 4.1: Let $\bar{\mathbf{u}}$ a conical intersection between λ_j and λ_{j+1}. Then there exists a suitably small neighborhood U of $\bar{\mathbf{u}}$ and $C>0$ such that

$$\lambda_{j+1}(\mathbf{u})-\lambda_j(\mathbf{u})\geq C|\mathbf{u}-\bar{\mathbf{u}}|,\ \forall \mathbf{u}\in U. \tag{11}$$

Let us now define the following matrices, which allow to introduce a further characterization of conical intersections and which play an important role for our strongest controllability results obtained in the cases **(R)** and **(C)**.

Definition 4.2: In the case **(R)** we define the *conicity matrix associated with* $(\psi_1,\psi_2)\in\mathcal{H}^{\mathbb{R}}\times\mathcal{H}^{\mathbb{R}}$ as

$$\mathcal{M}(\psi_1,\psi_2)=\begin{pmatrix} \langle\psi_1,H_1\psi_2\rangle & \frac{1}{2}\big(\langle\psi_2,H_1\psi_2\rangle-\langle\psi_1,H_1\psi_1\rangle\big)\\ \langle\psi_1,H_2\psi_2\rangle & \frac{1}{2}\big(\langle\psi_2,H_2\psi_2\rangle-\langle\psi_1,H_2\psi_1\rangle\big)\end{pmatrix}.$$

If **(C)** holds, then the *conicity matrix associated with* $(\psi_1,\psi_2)\in\mathcal{H}\times\mathcal{H}$ is defined as

$$\mathcal{M}(\psi_1,\psi_2)=$$
$$\begin{pmatrix}\langle\psi_1,H_1\psi_2\rangle & \langle\psi_1,H_1\psi_2\rangle^* & \langle\psi_2,H_1\psi_2\rangle-\langle\psi_1,H_1\psi_1\rangle\\ \langle\psi_1,H_2\psi_2\rangle & \langle\psi_1,H_2\psi_2\rangle^* & \langle\psi_2,H_2\psi_2\rangle-\langle\psi_1,H_2\psi_1\rangle\\ \langle\psi_1,H_3\psi_2\rangle & \langle\psi_1,H_3\psi_2\rangle^* & \langle\psi_2,H_3\psi_2\rangle-\langle\psi_1,H_3\psi_1\rangle\end{pmatrix}.$$

Lemma 4.3: If **(R)** holds, the function $(\psi_1,\psi_2)\mapsto|\det\mathcal{M}(\psi_1,\psi_2)|$ is invariant under orthogonal transformations of the argument, that is if $(\widehat{\psi}_1,\widehat{\psi}_2)^T=\mathcal{O}(\psi_1,\psi_2)^T$ for a pair ψ_1,ψ_2 of orthonormal elements of $\mathcal{H}^{\mathbb{R}}$ and $\mathcal{O}\in\mathsf{O(2)}$, then one has $|\det\mathcal{M}(\widehat{\psi}_1,\widehat{\psi}_2)|=|\det\mathcal{M}(\psi_1,\psi_2)|$. If **(C)** holds, then $\det\mathcal{M}(\psi_1,\psi_2)$ is purely imaginary and the function $(\psi_1,\psi_2)\mapsto\det\mathcal{M}(\psi_1,\psi_2)$ is invariant under unitary transformation of the argument, that is if $(\widehat{\psi}_1,\widehat{\psi}_2)^T=\mathbb{U}(\psi_1,\psi_2)^T$ for a pair ψ_1,ψ_2 of orthonormal elements of $\mathcal{H}$ and $\mathbb{U}\in\mathsf{U(2)}$, then one has $\det\mathcal{M}(\widehat{\psi}_1,\widehat{\psi}_2)=\det\mathcal{M}(\psi_1,\psi_2)$.

The following result characterizes conical intersections in terms of the conicity matrix.

Proposition 4.4: Assume that **(R)** or **(C)** holds and that $\{\lambda_j,\lambda_{j+1}\}$ is a separated discrete spectrum with $\lambda_j(\bar{\mathbf{u}})=\lambda_{j+1}(\bar{\mathbf{u}})$. Let $\{\psi_1,\psi_2\}$ be an orthonormal basis of the eigenspace associated with the double eigenvalue, with $\psi_1,\psi_2\in\mathcal{H}^{\mathbb{R}}$ in the **(R)** case. Then $\bar{\mathbf{u}}$ is a conical intersection if and only if $\mathcal{M}(\psi_1,\psi_2)$ is nonsingular.

As noticed above, for any analytic curve that reaches a conical intersection it is possible to choose analytic eigenstates along the curve. A peculiarity of conical intersections is that, when approaching the singularity from different directions, the eigenstates corresponding to the intersecting eigenvalues have different limits. Calling ϕ_j^0,ϕ_{j+1}^0 be the limits as $t\to0^+$ of the eigenstates $\phi_j(r_0(t)),\phi_{j+1}(r_0(t))$ along a straight line $r_0(t)=\mathbf{u}+t\mathbf{v}_0$ for some unit vector $\mathbf{v}_0$, and $\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}}$ the limit basis along the straight line $r_{\mathbf{v}}(t)=\mathbf{u}+t\mathbf{v}$, we can relate them by the following transformation, up to some phases for $\phi_j^{\mathbf{v}}$ and $\phi_{j+1}^{\mathbf{v}}$:

$$\begin{pmatrix}\phi_j^{\mathbf{v}}\\ \phi_{j+1}^{\mathbf{v}}\end{pmatrix}=\begin{pmatrix}\cos\boldsymbol{\Xi} & e^{-i\beta}\sin\boldsymbol{\Xi}\\ -e^{i\beta}\sin\boldsymbol{\Xi} & \cos\boldsymbol{\Xi}\end{pmatrix}\begin{pmatrix}\phi_j^0\\ \phi_{j+1}^0\end{pmatrix}. \tag{12}$$

Using (10), it is easy to see that the parameters $\boldsymbol{\Xi}=\boldsymbol{\Xi}(\mathbf{v})$ and $\beta=\beta(\mathbf{v})$ satisfy the following equations:

$$\tan 2\boldsymbol{\Xi}(\mathbf{v})=\frac{2|\langle\phi_j^0,H_{\mathbf{v}}\phi_{j+1}^0\rangle|}{\langle\phi_j^0,H_{\mathbf{v}}\phi_j^0\rangle-\langle\phi_{j+1}^0,H_{\mathbf{v}}\phi_{j+1}^0\rangle} \tag{13}$$
$$\beta(\mathbf{v})=\arg\langle\phi_j^0,H_{\mathbf{v}}\phi_{j+1}^0\rangle, \tag{14}$$

where $H_{\mathbf{v}}=\sum_{i=1}^m H_iv_i$.

Remark 4.5: It can be seen that not all the solutions of (13)-(14) provide the correct transformation (12). Nevertheless, let $\mathbf{v}_0,\mathbf{v}_1$ be two unit vectors and $\mathbf{w}(s)$, $s\in[0,\bar{s}]$, be a curve joining $\mathbf{v_0}$ to $\mathbf{v}_1$ such that $\mathbf{w}(s)\notin\{\mathbf{v}_0,-\mathbf{v}_0\}$ for every $s\in(0,\bar{s})$; for conical intersections, it is possible to associate with such a curve a continuous solution $(\boldsymbol{\Xi}(\mathbf{w}(s)),\beta(\mathbf{w}(s)))$ of (13)-(14) with $\boldsymbol{\Xi}(\mathbf{v}_0)=0$ and compatible with (12). It is easy to see that $\boldsymbol{\Xi}(\mathbf{w}(s))\in[-\pi/2,0]$ for $s\in[0,\bar{s}]$ from which one deduces that the final value $\boldsymbol{\Xi}(\mathbf{v}_1)=\boldsymbol{\Xi}(\mathbf{w}(\bar{s}))$ is independent of the chosen path and continuously depends on $\mathbf{v}_1$. In particular it turns out that $\boldsymbol{\Xi}(-\mathbf{v}_0)=-\pi/2$. Similarly, one can show that $\beta(\mathbf{v}_1)=\beta(\mathbf{w}(\bar{s}))$ is independent of the chosen path and continuous outside $\{\mathbf{v}_0,-\mathbf{v}_0\}$. Note that the fact that β is discontinuous at $-\mathbf{v}_0$ implies that the corresponding limit basis $(\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}})$ has a discontinuity at $-\mathbf{v}_0$.

V. A SPREAD CONTROLLABILITY RESULT

Our first result states that spread controllability holds for a class of systems having pairwise conical intersections, providing in addition an estimate of the controllability time. As a byproduct of the proof, we will also get an explicit characterization of the motion planning strategy (the path $\gamma(\cdot)$ below).

Theorem 5.1: Let $H(\mathbf{u})=H_0+\sum_{i=1}^m u_iH_i$ satisfy hypothesis **(H0)**. Let $\Sigma:\mathbf{u}\mapsto\{\lambda_0(\mathbf{u}),\dots,\lambda_k(\mathbf{u})\}$ be a separated discrete spectrum on $\omega\subset\mathbb{R}^m$ and assume that there exist conical intersections $\mathbf{u}_j\in\omega$, $j=0,\dots,k-1$, between the eigenvalues λ_j,λ_{j+1}, with $\lambda_l(\mathbf{u}_j)$ simple if $l\neq j,j+1$. Then, for every $\mathbf{u}^0$ and $\mathbf{u}^1$ such that $\Sigma(\mathbf{u}^0)$ and $\Sigma(\mathbf{u}^1)$ are non-degenerate, for every $\bar{\phi}\in\{\phi_0(\mathbf{u}^0),\dots,\phi_k(\mathbf{u}^0)\}$, and $p\in[0,1]^{k+1}$ such that $\sum_{l=0}^k p_l^2=1$, there exist $C>0$ and a continuous control $\gamma(\cdot):[0,1]\to\mathbb{R}^m$ with $\gamma(0)=\mathbf{u}^0$ and $\gamma(1)=\mathbf{u}^1$, such that for every $\varepsilon>0$

$$\|\psi(1/\varepsilon)-\sum_{j=0}^k p_je^{i\vartheta_j}\phi_j(\mathbf{u}^1)\|\leq C\sqrt{\varepsilon}, \tag{15}$$

where $\psi(\cdot)$ is the solution of (2) with $\psi(0)=\bar{\phi}$, $\mathbf{u}(t)=\gamma(\varepsilon t)$, and $\vartheta_0,\dots,\vartheta_k\in\mathbb{R}$ are some phases depending on ε and γ. In particular, (2) is approximately spread controllable on Σ.

The control strategy consists in constructing piecewise smooth paths that pass through conical intersections making suitable corners. While far from a conical intersection, we can use an adiabatic approximation that separates all the levels in Σ, and therefore the occupation probabilities of the energy levels are approximately conserved. When in a neighborhood of a conical intersection (to fix the ideas, between the eigenvalues λ_j and λ_{j+1}), we will treat the two intersecting levels together, by means of (7). We then consider the effective Hamiltonian and its associated evolution operator $U_{\text{eff}}^{\varepsilon}$. The key point is that there exists some phases (depending on ε) $\vartheta_j,\vartheta_{j+1}$ such that

$$\|U_{\text{eff}}^{\varepsilon}(0,\tau_0)-\begin{pmatrix}e^{i\vartheta_j} & 0\\ 0 & e^{i\vartheta_{j+1}}\end{pmatrix}\|\leq C\sqrt{\varepsilon},$$

and a similar inequality holds for $U_{\text{eff}}^{\varepsilon}(\tau_0,1)$. This fact can be shown with explicit computations (see e.g. [8]). We remark that the term $\sqrt{\varepsilon}$ is due to the presence of intersecting eigenvalues (see [8] and also [19, Corollary 2.5] for a similar result). The spreading of occupation probabilities induced by the corner at the singularity is described by the following proposition.

Proposition 5.2: Let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues λ_j,λ_{j+1}, and let $\gamma:[0,1]\to\omega$ be the curve defined as

$$\gamma(\tau)=\begin{cases}\bar{\mathbf{u}}+(\tau_0-\tau)\mathbf{v}_0 & \tau\in[0,\tau_0]\\ \bar{\mathbf{u}}+(\tau-\tau_0)\mathbf{v} & \tau\in[\tau_0,1].\end{cases}$$

Let ϕ_j^0, ϕ_{j+1}^0 be limits as $\tau \to \tau_0^-$ of the eigenstates $\phi_j(\gamma(\tau)), \phi_{j+1}(\gamma(\tau))$, respectively. Then there exists $C > 0$ such that, for any $\varepsilon > 0$,

$$\|\psi(1/\varepsilon) - p_1 e^{i\vartheta_j}\phi_j(\gamma(1)) - p_2 e^{i\vartheta_{j+1}}\phi_{j+1}(\gamma(1))\| \le C\sqrt{\varepsilon} \quad (16)$$

where $\vartheta_j,\ \vartheta_{j+1} \in \mathbb{R}$, $\psi(\cdot)$ is the solution of equation (2) with $\psi(0) = \phi_j(\gamma(0))$ corresponding to the control $\mathbf{u} : [0, 1/\varepsilon] \to \omega$ defined by $\mathbf{u}(t) = \gamma(\varepsilon t)$,

$$p_1 = |\cos(\boldsymbol{\Xi}(\mathbf{v}))|,\ \ p_2 = |\sin(\boldsymbol{\Xi}(\mathbf{v}))|,$$

and $\boldsymbol{\Xi}(\cdot)$ is defined as in equation (13) and Remark 4.5.

Remark 5.3: For control purposes, it is interesting to consider the case in which the initial probability is concentrated in the first level, the final occupation probabilities p_1^2 and p_2^2 are prescribed.

Choosing $\eta \in [0, \pi/2]$ such that $(p_1, p_2) = (\cos\eta, \sin\eta)$, we select the outcoming direction $\mathbf{v}$ in such a way that it satisfies

$$\boldsymbol{\Xi}(\mathbf{v}) = \pm\eta.$$

Thanks to Remark 4.5, this is always possible.

VI. Non-mixing curves

The purpose of this section is to improve the controllability results in the cases **(R)** and **(C)**. Throughout the section we assume, without loss of generality, that $\{\lambda_j, \lambda_{j+1}\}$ is a separated discrete spectrum on an open domain ω and that $0 \in \omega$ is the only conical intersection between the eigenvalues.

Following Section III-A, the effective Hamiltonian $H_{\text{eff}}^{\varepsilon}$, defined as in (7), (approximately) describes the dynamics in the eigenspaces associated with λ_j, λ_{j+1}, for $\mathbf{u}$ slowly varying in ω. When integrating the effective Hamiltonian, the off-diagonal terms in (7) induce a (a priori) non-negligible probability transfer between the two levels, which is taken into account in the estimate (15) by the term $O(\sqrt{\varepsilon})$.

Thus, to improve the precision of the result, we need to kill the off-diagonal terms in the effective Hamiltonian. In order to do that, we choose some special trajectories in ω along which the term $\langle \phi_j, \dot\phi_{j+1}\rangle$ is null. Here and in the following we use the notation $\dot\phi = \dot\phi(\gamma(\cdot))$ to denote $\frac{d}{dt}(\phi(\gamma(\cdot)))$.

We treat the cases **(R)** and **(C)** separately.

(R) We consider trajectories satisfying the following system

$$\begin{cases} \dot u_1 = -\langle \phi_j, H_2 \phi_{j+1}\rangle \\ \dot u_2 = \langle \phi_j, H_1\phi_{j+1}\rangle. \end{cases} \quad (17)$$

Notice that the right-hand side of (17) can be taken real-valued under the current hypotheses. It is defined up to a sign, because of the freedom in the choice of the sign of the eigenstates. Nevertheless, locally around points where $\lambda_j \neq \lambda_{j+1}$, it is possible to choose the sign in such a way that the right-hand side of (17) is smooth, and, from equation (9), we see that $\langle \phi_j(\gamma(t)), \dot\phi_{j+1}(\gamma(t))\rangle = 0$ along any integral curve γ of (17). Let now $\mathrm{Gr}_2(\mathcal{H}^{\mathbb{R}})$ be the 2-Grassmannian of $\mathcal{H}^{\mathbb{R}}$, i.e. the set of all two-dimensional subspaces of $\mathcal{H}^{\mathbb{R}}$. This set has a natural structure of a metric space defined by the distance $d(W_1, W_2) = \|P_{W_1} - P_{W_2}\|$, where P_{W_1}, P_{W_2} are the orthogonal projections on the two-dimensional subspaces W_1, W_2. Lemma 4.3 allows us to define the function $\hat F : \mathrm{Gr}_2(\mathcal{H}^{\mathbb{R}}) \to \mathbb{R}$ as $\hat F(W) = |\det \mathcal{M}(v_1, v_2)|$, where $\{v_1, v_2\}$ is any orthonormal basis of $W \in \mathrm{Gr}_2(\mathcal{H}^{\mathbb{R}})$. It is easy to see that $\hat F$ is continuous.

Let $P_{\mathbf{u}}$ be the spectral projection associated with the pair $\{\lambda_j(\mathbf{u}), \lambda_{j+1}(\mathbf{u})\}$. We know from Section III-B that $P_{\mathbf{u}}$ is analytic on ω. Therefore $\mathbf{u} \mapsto P_{\mathbf{u}}\mathcal{H} \cap \mathcal{H}^{\mathbb{R}}$ is continuous in $\mathrm{Gr}_2(\mathcal{H}^{\mathbb{R}})$. Let now $F(\mathbf{u}) := |\det \mathcal{M}(\phi_j(\mathbf{u}), \phi_{j+1}(\mathbf{u}))|$. Since $F(\mathbf{u}) = \hat F(P_{\mathbf{u}}\mathcal{H} \cap \mathcal{H}^{\mathbb{R}})$ and by Proposition 4.4 we get the following result.

Lemma 6.1: The function $\mathbf{u} \mapsto F(\mathbf{u})$ is well defined and continuous in ω. In particular F is different from 0 in a neighborhood of $\mathbf{u} = 0$.

Without loss of generality, we assume from now on that F is different from zero on ω.

Lemma 6.2: There exists a $\mathcal{C}^\infty$ choice of the right-hand side of (17) in $\omega \setminus \{0\}$ such that, if $\mathbf{u}(\cdot)$ is a corresponding solution, then

$$\frac{d}{dt}\Big[\lambda_{j+1}(\mathbf{u}(t)) - \lambda_j(\mathbf{u}(t))\Big] = -2F(\mathbf{u}(t)) \quad (18)$$

on $\omega \setminus \{0\}$.

We now define the *non-mixing field*, denoted by $\mathcal{X}_P$, as the smooth vector field on $\omega \setminus \{0\}$ identified by the preceding lemma. Its integral curves are $\mathcal{C}^\infty$ in $\omega \setminus \{0\}$. Moreover, its norm is equal to the norm of the first row of $\mathcal{M}(\phi_j, \phi_{j+1})$, and therefore bounded both from above and from below by positive constants in $\omega \setminus \{0\}$.

By considering $\lambda_{j+1}(\mathbf{u}) - \lambda_j(\mathbf{u})$ as a local Lyapunov function, the above results lead to the following proposition.

Proposition 6.3: There exists a punctured neighborhood U of 0 such that all the integral curves of $\mathcal{X}_P$ starting from U reach the origin in finite time.

The integral curves of non-mixing field turn out to be smooth even at the singularity (for technical details, see [8]).

Proposition 6.4: Let $\gamma : [-\eta, 0] \to \omega$ be an integral curve of $\mathcal{X}_P$ with $\gamma(0) = 0$. Then $\gamma(\cdot)$ and the eigenstates $\phi_j(\gamma(\cdot)), \phi_{j+1}(\gamma(\cdot))$ are $\mathcal{C}^\infty$ on $[-\eta, 0]$.

The following result is crucial to our controllability strategy.

Proposition 6.5: For every unit vector $\mathbf{w}$ in $\mathbb{R}^2$ there exists an integral curve $\gamma : [-\eta, 0] \to \omega$ of $\mathcal{X}_P$ with $\gamma(0) = 0$ such that

$$\lim_{t \to 0^-} \frac{\dot\gamma(t)}{\|\dot\gamma(t)\|} = \mathbf{w}.$$

By concatenating integral curves of the non-mixing field, we construct paths that realize the transitions with a precision of the order ε. This allows us to state the following result:

Theorem 6.6: Consider the case **(R)**, and let the hypotheses of Theorem 5.1 hold. Then for every $\mathbf{u}^0$ and $\mathbf{u}^1$ such that $\Sigma(\mathbf{u}^0)$ and $\Sigma(\mathbf{u}^1)$ are non-degenerate, for every $\bar\phi \in \{\phi_0(\mathbf{u}^0), \ldots, \phi_k(\mathbf{u}^0)\}$, and $p \in [0,1]^{k+1}$ such that $\sum_{l=0}^k p_l^2 = 1$, there exist $C > 0$ and a continuous control $\gamma(\cdot) : [0,1] \to \mathbb{R}^2$ with $\gamma(0) = \mathbf{u}^0$ and $\gamma(1) = \mathbf{u}^1$, such that for every $\varepsilon > 0$

$$\|\psi(1/\varepsilon) - \sum_{j=0}^k p_j e^{i\vartheta_j}\phi_j(\mathbf{u}^1)\| \le C\varepsilon, \quad (19)$$

where $\psi(\cdot)$ is the solution of (2) with $\psi(0) = \bar\phi$, $\mathbf{u}(t) = \gamma(\varepsilon t)$, and $\vartheta_0, \ldots, \vartheta_k \in \mathbb{R}$ are some phases depending on ε and γ.

Remark 6.7: The phases $\vartheta_0, \ldots, \vartheta_k$ may, in principle, be computed explicitly. In fact, they are sums of terms of the form $\frac{1}{\varepsilon}\int_{s_l}^{s_{l+1}} \lambda_j(\gamma(s))\, ds$, where $\gamma|_{[s_l, s_{l+1}]}$ are the pieces of the path γ between two successive passages through conical intersections. Moreover, if at the final point $\mathbf{u}^0$ (or at any other point of the chosen path) all the ratios $\frac{\lambda_j(\mathbf{u}^0)}{\lambda_l(\mathbf{u}^0)}$, $l \neq j$, $j, l = 0, \ldots, k$, are not rational, then, by stopping at $\mathbf{u}^0$ for a long enough time, one can approximately recover every final value of $(\vartheta_0, \ldots, \vartheta_k)$ (the rational independence of the eigenvalues guarantees that the set of points $(\vartheta_0, \ldots, \vartheta_k)$ attainable from any initial configuration is dense in the k-dimensional torus). Thus this method allows to (approximately) induce any transition from an eigenstate relative to the eigenvalues in Σ to any other state belonging to the sum of eigenspaces relative to the eigenvalues in Σ. Notice however that the computation of the final phases is very sensitive to variations of ε and to errors in the computation of the eigenvalues, and also approximate recovering of the desired phases could need a very large time, leading to important computational errors. Therefore this controllability strategy seems to be essentially unfeasible in practice.

We conclude the study of the case **(R)** with a result of structural stability of conical intersections.

Theorem 6.8: Assume $\bar{\mathbf{u}}$ is a conical intersection between the eigenvalues λ_j and λ_{j+1} for an Hamiltonian $H(\mathbf{u}) = H_0 + u_1 H_1 + u_2 H_2$ in the case **(R)**. Assume moreover that $\mathbf{u} \mapsto \{\lambda_j(\mathbf{u}), \lambda_{j+1}(\mathbf{u})\}$ is a separated discrete spectrum in a neighborhood of $\bar{\mathbf{u}}$. Then for every $\varepsilon > 0$ there exists $\delta > 0$ such that, if $\hat{H}(\mathbf{u}) = \hat{H}_0 + u_1 \hat{H}_1 + u_2 \hat{H}_2$ is in the case **(R)** and

$$\|\hat{H}_0 - H_0\| + \|\hat{H}_1 - H_1\| + \|\hat{H}_2 - H_2\| \leq \delta, \qquad (20)$$

then the operator $\hat{H}(\mathbf{u})$ admits a conical intersection of eigenvalues at $\hat{\mathbf{u}}$, with $|\bar{\mathbf{u}} - \hat{\mathbf{u}}| \leq \varepsilon$.

(C) The results obtained in the case **(R)** can be partially adapted to the case **(C)**. We only give a sketch of the necessary modifications.

Similarly to the above construction, we can define the function $\mathbf{u} \mapsto \det \mathcal{M}(\phi_j(\mathbf{u}), \phi_{j+1}(\mathbf{u}))$, where $\phi_j(\mathbf{u}), \phi_{j+1}(\mathbf{u})$ are eigenstates relative to the intersecting eigenvalues. We can prove the analogue of Lemma 6.1, that is, the previous function is continuous and therefore it has constant sign in a neighbourhood of the conical intersection.

Let us now introduce the following vector

$$\boldsymbol{m}(\psi_1, \psi_2) = (\langle \psi_1, H_1 \psi_2 \rangle, \langle \psi_1, H_2 \psi_2 \rangle, \langle \psi_1, H_3 \psi_2 \rangle)^T, \qquad (21)$$

where $\psi_1, \psi_2 \in \mathcal{H}$ and denote its components $\langle \psi_1, H_i \psi_2 \rangle$ as m_i. Moreover we call

$$\begin{aligned} \boldsymbol{m}^*(\psi_1, \psi_2) &= (m_1^*, m_2^*, m_3^*)^T \\ \mathfrak{Re}\boldsymbol{m} &= (\mathfrak{Re} m_1, \mathfrak{Re} m_2, \mathfrak{Re} m_3)^T \\ \mathfrak{Im}\boldsymbol{m} &= (\mathfrak{Im} m_1, \mathfrak{Im} m_2, \mathfrak{Im} m_3)^T. \end{aligned}$$

It is easy to see that the real vector

$$\begin{aligned} X(\psi_1, \psi_2) &= \frac{\boldsymbol{m}(\psi_1, \psi_2) \times \boldsymbol{m}^*(\psi_1, \psi_2)}{2i} \\ &= (\mathfrak{Im}(m_2 m_3^*), \mathfrak{Im}(m_3 m_1^*), \mathfrak{Im}(m_1 m_2^*))^T, \end{aligned} \qquad (22)$$

where $\times$ denotes the cross product, is orthogonal to both $\mathfrak{Im}\boldsymbol{m}$ and $\mathfrak{Re}\boldsymbol{m}$.

Remark 6.9: Let us remark that the vector $X(\psi_1, \psi_2)$ is invariant under phase changes in the argument, that is $X(\psi_1, \psi_2) = X(e^{i\beta_1}\psi_1, e^{i\beta_2}\psi_2)$. Notice however that $X(\psi_1, \psi_2) = -X(\psi_2, \psi_1)$.

Consider now the vector field $\mathcal{X}_P(\mathbf{u}) = X(\phi_j(\mathbf{u}), \phi_{j+1}(\mathbf{u}))$, and call it the non-mixing field. It turns out that it is well defined and smooth in a punctured neighborhood of the conical intersection, and, because of (9) and (22), we have $\langle \phi_j, \dot{\phi}_{j+1} \rangle = 0$ along its integral curves. Moreover, since

$$\left\langle X(\psi_1, \psi_2), \begin{pmatrix} \langle \psi_2, H_1 \psi_2 \rangle - \langle \psi_1, H_1 \psi_1 \rangle \\ \langle \psi_2, H_2 \psi_2 \rangle - \langle \psi_1, H_2 \psi_1 \rangle \\ \langle \psi_2, H_3 \psi_2 \rangle - \langle \psi_1, H_3 \psi_1 \rangle \end{pmatrix} \right\rangle = \frac{1}{2i} \det \mathcal{M}(\psi_1, \psi_2),$$

we can conclude as in Proposition 6.3 that there is a global choice of the sign of $\mathcal{X}_P(\mathbf{u})$ such that all its integral curves starting from a punctured neighborhood of the conical intersection reach it in finite time.

The other technical results concerning the non-mixing field and its integral curves, stated for the case **(R)**, still hold true for the case **(C)**. The proofs can be derived from those contained in [8], after an adaptation to the current framework. This means that we can construct the effective Hamiltonian along the integral curves of the non-mixing field that go through the conical intersection, thus controlling the spreading of the occupation probability between the two levels involved. In particular, Theorem 6.6, remains true in the case **(C)**.

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